

Table 1. Observed and calculated structure factors for mozartite
mozlt: 100K , mozrt: 300K, mozht: 500K.

'Orthorhombic Jahn-Teller distortion and Si-OH in mozartite....'
Nyfeler et al.

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR

PAGE 1

Table with columns H, K, L, FO, FC, S for three different groups of reflections. Each row contains numerical values representing observed and calculated structure factors and their differences.

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR

PAGE 2

Table with columns H, K, L, FO, FC, S and rows of numerical data representing structure factors. Each row contains three sets of six columns.

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR MOZARTITE, 12.12.95, RT

Table with 27 columns (H, K, L, FO, FC, S for four groups) and many rows of numerical data representing structure factors and their differences.

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR MOZARTITE 200 C 20.1.96

Table with 30 columns (H, K, L, FO, FC, S) and approximately 90 rows of numerical data representing structure factors.

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR MOZARTITE 200 C 20.1.96

PAGE 5

H	K	L	FO	FC	S	H	K	L	FO	FC	S	H	K	L	FO	FC	S	H	K	L	FO	FC	S						
2	7	11	37	37	1	6	2	12	20	20	1	-3	7	12	8	6	-2	5	3	13	12	12	1	0	2	14	19	20	1
3	7	11	15	15	1	-6	3	12	7	4	-4	-2	7	12	10	4	-3	-5	4	13	5	6	-6	1	2	14	25	26	1
4	7	11	5	8	-6	-5	3	12	3	3	-10	-1	7	12	10	10	1	-3	4	13	2	1	-8	2	2	14	24	24	1
5	7	11	10	13	-3	-4	3	12	10	8	1	0	7	12	10	2	-3	-2	4	13	11	1	-3	3	2	14	25	24	1
-3	8	11	10	12	2	-2	3	12	2	2	-9	1	7	12	10	10	1	-1	4	13	10	5	-3	4	2	14	15	16	1
-2	8	11	7	3	-4	0	3	12	10	11	1	2	7	12	4	4	-18	0	4	13	6	4	-5	-4	3	14	8	6	-4
-1	8	11	17	15	1	1	3	12	4	3	-7	-1	8	12	5	6	-7	1	4	13	7	5	-5	-3	3	14	10	8	1
1	8	11	17	16	1	2	3	12	5	3	-6	0	8	12	25	25	1	3	4	13	7	0	-4	-2	3	14	8	7	-4
2	8	11	10	3	-3	3	3	12	6	5	-5	1	8	12	6	6	-5	-4	5	13	13	14	1	-1	3	14	8	7	-4
3	8	11	13	11	1	4	3	12	9	8	-2	2	8	12	9	4	-2	-3	5	13	8	7	-4	0	3	14	4	6	-8
-2	9	11	30	28	1	6	3	12	6	4	-6	1	0	13	13	13	1	-2	5	13	21	21	1	1	3	14	6	6	-5
-1	9	11	16	15	1	-6	4	12	30	30	1	3	0	13	9	7	-2	-1	5	13	9	10	-3	2	3	14	9	7	-3
1	9	11	15	15	1	-4	4	12	13	13	1	4	0	13	9	3	-3	0	5	13	13	14	1	3	3	14	9	8	-2
2	9	11	29	28	1	-3	4	12	15	15	1	5	0	13	10	5	-3	1	5	13	8	10	-4	4	3	14	6	6	-6
0	0	12	41	41	1	-2	4	12	44	45	1	-5	1	13	6	4	-4	2	5	13	23	21	1	-3	4	14	9	4	-3
2	0	12	8	3	-3	-1	4	12	8	7	-3	-4	1	13	29	30	1	3	5	13	7	7	-4	-2	4	14	6	7	-5
3	0	12	4	1	-6	0	4	12	12	10	1	-3	1	13	7	11	-4	4	5	13	11	14	1	0	4	14	35	36	1
4	0	12	32	33	1	1	4	12	8	6	-4	-2	1	13	17	17	1	-3	6	13	8	6	-2	2	4	14	5	7	-7
5	0	12	8	10	-2	2	4	12	47	45	1	-1	1	13	4	10	-7	0	6	13	12	14	1	-2	5	14	9	9	-4
6	0	12	7	5	-2	3	4	12	16	15	1	0	1	13	34	33	1	1	6	13	7	7	-4	-1	5	14	6	9	-5
-6	1	12	2	8	-8	4	4	12	11	12	1	1	1	13	7	9	-4	2	6	13	6	7	-5	0	5	14	10	9	2
-3	1	12	8	3	-3	6	4	12	29	30	1	2	1	13	16	16	1	0	7	13	21	21	1	1	5	14	9	8	-4
-2	1	12	5	8	-6	-5	5	12	8	11	-4	3	1	13	13	11	1	1	7	13	6	9	-5	0	6	14	16	17	1
-1	1	12	5	4	-6	-4	5	12	7	7	-2	4	1	13	30	31	1	1	0	14	12	11	1	1	0	15	6	2	-5
0	1	12	2	3	-8	-1	5	12	8	9	-2	-4	2	13	6	8	-5	2	0	14	42	43	1	2	0	15	7	4	-4
2	1	12	10	8	-3	0	5	12	11	10	-3	-1	2	13	7	2	-4	3	0	14	7	11	-3	3	0	15	6	1	-5
3	1	12	6	3	-4	1	5	12	9	9	-3	0	2	13	9	10	-2	4	0	14	10	10	1	-3	1	15	4	5	-18
4	1	12	3	5	-12	2	5	12	6	4	-5	2	2	13	6	5	-5	-4	1	14	9	11	2	-2	1	15	8	11	-4
6	1	12	10	8	1	3	5	12	6	5	-5	3	2	13	6	3	-4	-3	1	14	2	8	-8	-1	1	15	12	11	1
-6	2	12	19	20	1	4	5	12	6	7	-5	4	2	13	9	8	-3	-2	1	14	10	11	-3	0	1	15	29	28	1
-5	2	12	6	9	-9	5	5	12	7	11	-4	-5	3	13	14	13	1	-1	1	14	13	12	1	1	1	15	10	11	-3
-4	2	12	23	24	1	-4	6	12	17	18	1	-4	3	13	11	13	1	0	1	14	10	10	-3	2	1	15	13	12	1
-3	2	12	20	20	1	-3	6	12	18	16	1	-3	3	13	6	8	-5	1	1	14	11	12	-3	-2	2	15	9	3	-4
-2	2	12	24	24	1	-2	6	12	24	22	1	-2	3	13	32	33	1	2	1	14	12	11	1	2	2	15	6	3	-6
-1	2	12	18	19	1	-1	6	12	18	18	1	-1	3	13	9	13	-4	3	1	14	10	8	-3	-2	3	15	27	28	1
0	2	12	24	24	1	0	6	12	19	19	1	0	3	13	12	11	1	4	1	14	10	10	-3	-1	3	15	14	14	1
1	2	12	18	18	1	1	6	12	19	18	1	1	3	13	11	12	-3	-4	2	14	14	16	1	0	3	15	10	3	-3
2	2	12	26	25	1	2	6	12	23	22	1	2	3	13	33	33	1	-3	2	14	23	24	1	1	3	15	5	14	-7
3	2	12	19	20	1	3	6	12	16	16	1	3	3	13	4	9	-14	-2	2	14	22	23	1	2	3	15	28	28	1
4	2	12	23	23	1	4	6	12	18	18	1	4	3	13	13	14	1	-1	2	14	24	25	1	0	4	15	8	1	-4